J. Pure Appl. & Ind. Phys. Vol.3 (2), 128-132 (2013)

# Fracto Mechanoluminescence in Coloured Alkali Halide Crystals

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(Received on: February 14, 2013)

## ABSTRACT

In coloured alkali halide crystals the recombination of electrons with $V_2$-centres in the crystal may give rise to the delayed luminescence where the delay time will depend on the life time of the electrons in the shallow traps. The time dependence of the ML intensity in coloured alkali halide crystals, which suggest that there should be two peaks in the ML intensity versus time curves of the crystals, where one peak should be in the deformation region and the other should be in post deformation region in the crystals.

**Keywords:** Delayed luminescence and shallowtrap.

## INTRODUCTION

Luminescence induced during mechanical deformation of solids is known as mechanoluminescence (ML). It can be excited by rubbing, grinding, cutting, cleaving, shaking, scratching, compressing or crushing of solids. ML also appears during the deformation caused by the phase transition or growth of certain crystals as well as during separation of two dissimilar materials in contact. The ML likes mechanical, spectroscopic, electrical, structural and other properties of solids. A large number of organic, inorganic crystals and amorphous solids exhibit the phenomena of ML[1-4]. It is known that coloured alkali halide crystals exhibit intense ML during their plastic deformation[5].

The present paper reports that the fracto mechanoluminescence in coloured alkali halide crystals The theory is able to explain the efficiency, spectroscopy and the kinetics of ML.

## THEORY

In a crystal having $N_d$ dislocations of unit length per unit volume. If $V_d$ is the

average velocity of the dislocation, then in time dt each dislocation will move a distance $V_d dt$. If $r_F$ is the radius of interaction of a dislocation with F-centres, then the volume of interaction per unit time will be $N_d V_d r_F$. If $n_F$ is the density of F-centres, then the rate of interaction of dislocations with F-centres may be given by

$$g_i = N_d V_d r_F n_F = \frac{\dot{\varepsilon}}{b} r_F n_F \quad (1)$$

where $\dot{\varepsilon} = N_d V_d b$, and b is the Burgers vector.The rate equation for the change in number of electron in dislocation band is

$$\frac{dN_d}{dt} = \frac{M_o v_o}{H} \exp\left(\frac{-v_d}{v_o}\right) \exp(-\alpha t) \quad (2)$$

If $\lambda_d$ is the mean free path of dislocations, then the number of F-centres excited by a dislocation is $\lambda_d P_F n_F r_F$. Therefore, the rate of generation of electrons is

$$g = g_o \exp(-\alpha t) \quad (3)$$

where

$$g_o = \frac{1}{H} \lambda_d P_F n_F M_o v_o \exp\left(\frac{-v_d}{v_o}\right) \quad (4)$$

If $\alpha_1$ is the rate of transfer of electrons from dislocation band to other centers, then we have

$$d\Delta n_1 = g_o \exp(-\alpha t) dt - \alpha_1 \Delta n_1 dt \quad (5)$$

where $\Delta n_1$ is the concentration of electrons in the dislocation band at any time t,

Integrating equation (5) and taking $\Delta n_1 = 0$, at t = 0, we get

$$\Delta n_1 = \frac{g_o}{(\alpha - \alpha_1)} [\exp(-\alpha_1 t) - \exp(-\alpha t)] \quad (6)$$

Similarly the number of electron in shallow traps at any time t

$$\Delta n_2 = g_o \alpha_1'' \left[ \frac{\exp(-\alpha t)}{(\alpha - \alpha_1)(\alpha - \alpha_2)} - \frac{\exp(-\alpha_1 t)}{(\alpha - \alpha_1)(\alpha - \alpha_2)} + \frac{\exp(-\alpha_2 t)}{(\alpha - \alpha_2)(\alpha_1 - \alpha_2)} \right] \quad (7)$$

Luminescence is produced during the recombination of dislocation electrons with the centres containing holes and also during the release of electrons the shallow traps and their subsequent recombination with hole containing centre. Thus, the luminescence intensity I may be written as

$$I = \left[\alpha_1' \Delta n_1 \eta_1 + \alpha_2 \Delta n_2 \eta_2\right] \quad (8)$$

where $\eta_1$ and $\eta_2$ are the probability of radiative electron-hole recombination.

By substituting the value of $\Delta n_1$ and $\Delta n_2$ from equation (6) and (7) in equation (8) we get

$$I = g_o [A \exp(-\alpha t) - B \exp(\alpha_1 t) + C \exp(-\alpha_2 t)] \quad (9)$$

we assume $\alpha_1 > \alpha > \alpha_2$ for coloured alkali halide crystals

$$A = \frac{\eta_1 \alpha_1' \alpha - \eta_2 \alpha_1'' \alpha_2}{\alpha_1 \alpha} \quad (10)$$

$$B = \frac{\eta_1 \alpha_1^{'} \alpha_1 - \eta_2 \alpha_1^{''} \alpha_2}{\alpha_1^2} \qquad (11)$$

$$C = \frac{\eta_2 \alpha_1^{''} \alpha_2}{\alpha_1 \alpha} \qquad (12)$$

**ESTIMATION OF $t_{m_1}, I_{m_1}, t_{m_2}, I_{m_2}$ AND $I_T$**

During the deformation of crystals at high strain-rate, dislocations move with high velocity and it has been found that $\beta$ lies in between 1.2 and 1.5 for KCl crystal. In the experimental investigation being made in laboratory, for the highest value of $v_o = 280\,\text{cm sec}^{-1}$, and for the thickness for the crystal H = 0.1 c.m., the highest value of $\alpha = \frac{(\beta v_o)}{H}$, comes out to be $3 \times 10^3\,\text{sec}^{-1}$. $\alpha_1$ is the rate constant for the recombination and it is given by

$$\alpha_1 = \sigma_1 N_1 v_d$$

where $\sigma_1$ and $N_1$ are the capture cross-section and density of the recombination centre (holes), respectively and $v_d$ is the velocity of the dislocation electrons which is equal to the velocity of dislocation. For $N_1 = 10^{17}\,\text{cm}^{-3}$, $\sigma_1 = 10^{-15}\,\text{cm}^2$ and $v_d \approx 10^4 - 10^5\,\text{cm s}^{-1}$, in the case of impulsive deformation $\alpha_1$ comes out to be nearly equal to $10^6 - 10^7\,\text{sec}^{-1}$.As $\alpha_2$ is the rate constant for the detrapping of the shallow traps, its value will depend on the trap-depth and the temperature of crystals.

**(i) Estimation of $t_{m_1}$**

For $\alpha_1 > \alpha > \alpha_2$, $\alpha_1^{'} \approx \alpha_1$, $\alpha_1^{''} < \alpha_1^{'}$ and $\eta_1 \geq \eta_2$, and value of A and B are much greater than C. equations (10), (11) and (12). For low value of t, $\exp(-\alpha_2 t) \approx 1$, thus we can neglect the term, $C \exp(-\alpha_2 t)$ in equation (9) and for maximum value of I, dI/dt is equal to zero, taking logarithm on both the sides and substituting $t = t_{m_1}$, and the values of A and B from equations (10) and (11) in the above equation, we get

$$t_{m_1} \approx \frac{1}{\alpha_1} \text{In}\left(\frac{\alpha_1}{\alpha}\right) \qquad (13)$$

$t_{m_1}$ should decreases slowly with increasing strain rate of the crystals.

**(ii) Estimation of $I_{m_1}$**

$$I_{m_1} \approx \frac{g_o \eta_1 \alpha_1^{'}}{\alpha_1} \qquad (14)$$

The above equation indicates that $I_{m_1}$ should increase with increasing strain-rate or impact velocity of the piston used to deform the crystal, as $g_o$ increases with increasing value of $v_o$

**(iii) Estimation of $t_{m_1}$**

For maximum value of I, $\frac{dI}{dt}$ is equal to zero, substituting the value of A and

C from equation (10) and (12), and substituting $t = t_m$, we get

$$t_{m_2} = \frac{1}{\alpha} \ln \frac{\eta_2 \alpha_1'' \alpha_2^2}{\eta_1 \alpha_1^1 \alpha^2} \tag{15}$$

Since the pre-exponential factor will be dominating, it is evident from equation (15) that $t_{m_2}$ should shift towards shorter time values with increasing strain-rate or impact velocity of the piston.

**(iv) Estimation of $I_{m_2}$**

$$I_{m_2} \approx \frac{g_o \eta_2 \alpha_1'' \alpha_2}{\alpha_1 \alpha} \tag{16}$$

As $g_o$ depends on the strain-rate, the above equation indicates that $I_{m_2}$ should increase with the strain-rate or impact velocity. However, as $\alpha$ also depends on the strain-rate, the value of $I_{m_2}$ should increase slowly with the strain rate as compared to that of $I_{m_1}$.

**(v) Estimation of total ML intensity $I_T$**

As $\alpha_1 >> \alpha >> \alpha_2$, $I_T$ is given by

$$I_T \approx \frac{g_o}{\alpha} \left[ \eta_1 \alpha_1' + \eta_2 \alpha_1'' \right] \tag{17}$$

It is evident from the above equation that $I_T$ should also increase with increasing strain-rate or impact velocity of the piston.

**COMPARISON BETWEEN THE THEORETICAL AND EXPERIMENTAL RESULTS**

Fig. 1 shows that both $I_{m_1}$ and $I_{m_2}$ increases non-linearly with increasing strain rate or impact velocity of the piston. $I_{m_1}$ does not saturate for higher values of the strain-rate or impact velocity $(v_o)$, however, $I_{m_2}$ gets saturated for higher values of $v_o$. It is evident from Fig. 2 that $I_T$ initially increases and then tends to attain a saturation value for higher values of the impact velocity. Fig. 3 shows that both $t_{m_1}$ and $t_{m_2}$ decreases with increasing impact velocity $v_o$ of the piston.

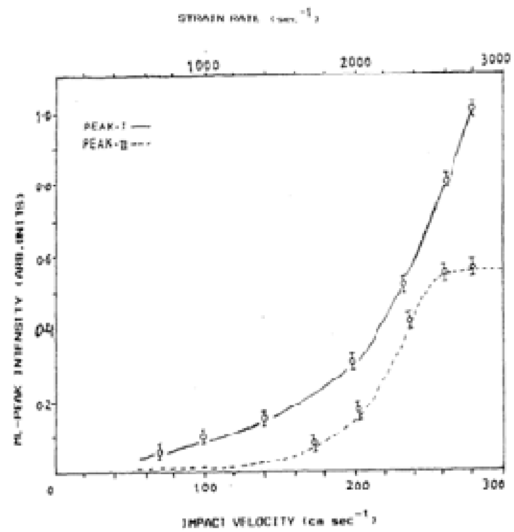


**Fig. 1Dependence of ML intensities of peak 1 and peak II or $\gamma$ -irradiated KCl crystals on different strain-rate or impact velocity impact velocity (crystal size $2 \times 2 \times 1 mm^3$, $n_F \approx 10^{17} cm^{-3}$ )**

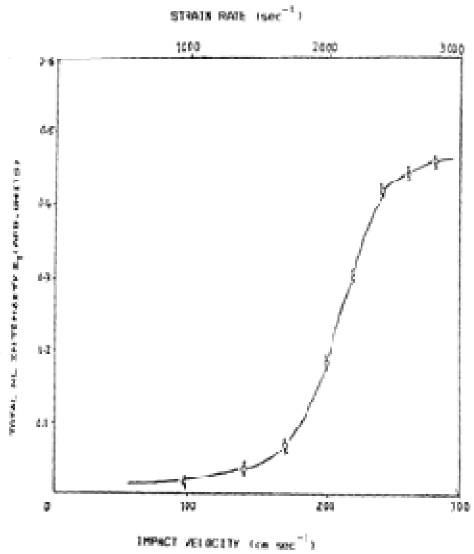

**Fig.2 Strain-rate or impact velocity dependence of total ML intensities $I_T$ of $\gamma$-irradiated KCl crystals (crystal size $2\times2\times1\,mm^3$, $n_F \approx 10^{17}\,cm^{-3}$)**

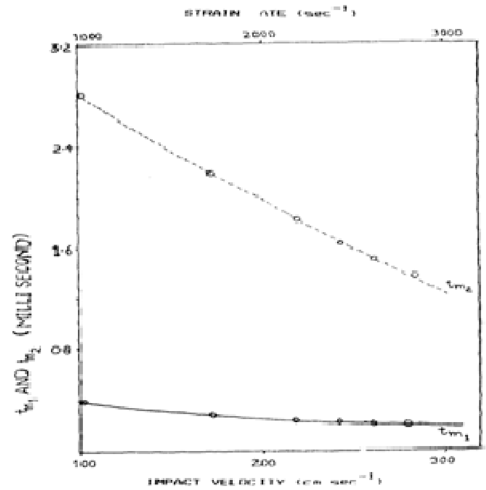

**Fig. 3 Dependence of $t_{m_1}$ and $t_{m_2}$ on strain-rate or impact velocity for KCl crystals (crystal size $2\times2\times1\,mm^3$, $n_F \approx 10^{17}\,cm^{-3}$)**

## CONCLUSION

The fracto mechanoluminescence in coloured alkali crystals has dislocation origin, in which the dislocation moving during deformation of the crystal capture electrons from the F-centers and transport them to the hole containing defect centers, where by the radiative electron-hole recombination gives rise to luminescence.

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